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NEWS 4 Feb 01 DKILIT now produced by FIZ Karlsruhe and has a new update frequency

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NEWS 7 Mar 22 TOXLIT no longer available

NEWS 8 Mar 22 TRCTHERMO no longer available NEWS 9 Mar 28 US Provisional Priorities searched with P in CA/CAplus

and USPATFULL

NEWS 10 Mar 28 LIPINSKI/CALC added for property searching in REGISTRY

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Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=>
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L1 STRUCTURE UPLOADED

=> d 11 L1 HAS NO ANSWERS

L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s 11 sss sam SAMPLE SEARCH INITIATED 16:07:49 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 2725 TO ITERATE

36.7% PROCESSED 1000 ITERATIONS (1 INCOMPLETE) 50 ANSWERS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
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PROJECTED ITERATIONS: 51371 TO 57629 PROJECTED ANSWERS: 4311 TO 6261

L2 50 SEA SSS SAM L1

=> d scan 12

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2,7-Naphthalenedisulfonic acid, 5-[[4-[[4-(cyanoamino)-6-[(3sulfophenyl)amino]-1,3,5-triazin-2-yl]amino]benzoyl]amino]-4-hydroxy-3-[[1sulfo-6-[[2-(sulfooxy)ethyl]sulfonyl]-2-naphthalenyl]azo]- (9CI)

MF C39 H30 N10 O20 S6

PAGE 1-A

PAGE 1-B

- oso₃H

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):49

- L2
- 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS [2,2'-Binaphthalene]-1,3',5,6'-tetrasulfonic acid, 8'-[[4-[[3-[[[2-1]]]]]])ΙN (ethenylsulfonyl)ethyl]amino]carbonyl]phenyl]amino]-6-fluoro-1,3,5-triazin-

2-yl]amino]-1'-hydroxy-, tetrasodium salt (9CI) MF $\,$ C34 H27 F N6 O16 S5 . 4 Na

•4 Na

- L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- Benzenesulfonic acid, 2,2'-(1,2-ethenediyl)bis[5-[[4-[[4-(aminocarbonyl)phenyl]amino]-6-[(2-methoxyethyl)amino]-1,3,5-triazin-2-yl]amino]-, disodium salt (9CI)
- MF C40 H42 N14 O10 S2 . 2 Na

PAGE 1-A

•2 Na

PAGE 1-B

$$\begin{array}{c|c} \text{NH-CH}_2\text{-CH}_2\text{-OMe} & \overset{\text{O}}{\underset{\text{N}}{\text{O}}} \\ & \overset{\text{N}}{\underset{\text{N}}{\text{NH-CH}_2}} \\ \end{array}$$

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzaldehyde, 3-nitro-, [4-[(4-nitrophenyl)amino]-6-[2,2,2-trifluoro-1-

09/891,750

(trifluoromethyl)ethoxy]-1,3,5-triazin-2-yl]hydrazone (9CI)
MF C19 H12 F6 N8 O5

$$_{\text{F}_3\text{C}-\text{CH}-\text{O}}^{\text{CF}_3}$$
 $_{\text{N}}^{\text{N}}$
 $_{\text{N}}^{\text{N}}$
 $_{\text{N}}^{\text{N}}$
 $_{\text{N}}^{\text{N}}$
 $_{\text{N}}^{\text{N}}$
 $_{\text{N}}^{\text{N}}$
 $_{\text{N}}^{\text{N}}$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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MF C21 H29 F3 N8 O2

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN Benzoic acid, 2-[(4,6-dimethoxy-2-pyrimidinyl)oxy]-6-[[4-(dimethylamino)-6-methoxy-1,3,5-triazin-2-yl]oxy]- (9CI)

MF C19 H20 N6 O7

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzoic acid, 4-[[4-chloro-6-[[4-(2-hydroxy-4-methoxy-5sulfobenzoyl)phenyl]amino]-1,3,5-triazin-2-yl]amino]-2-hydroxy-,
monosodium salt (9CI)

MF C24 H18 Cl N5 O9 S . Na

Na

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzenesulfonic acid, 2,2'-(1,2-ethenediyl)bis[5-[[4-[(4acetylphenyl)amino]-6-propoxy-1,3,5-triazin-2-yl]amino]-, disodium salt
(9CI)

MF C42 H42 N10 O10 S2 . 2 Na

•2 Na

PAGE 1-B

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzoic acid, 2,2'-[[6-[(2-hydroxyethyl)amino]-1,3,5-triazine-2,4diyl]bis[imino(6,13-dichloro-4,11-disulfo-10,3triphenodioxazinediyl)imino[6-[(2-hydroxyethyl)amino]-1,3,5-triazine-4,2diyl]imino]]bis- (9CI)

MF C65 H46 C14 N22 O23 S4

PAGE 1-A

PAGE 1-B

- **PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
- L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN Benzaldehyde, 2-hydroxy-3,5-dinitro-, [4-[(3,4-dimethylphenyl)amino]-6-[(4-nitrophenyl)amino]-1,3,5-triazin-2-yl]hydrazone (9CI)
- MF C24 H20 N10 O7

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS ITERATION INCOMPLETE
- IN 1,3,5-Triazin-2-amine, N-[4-(chlorodifluoromethoxy)phenyl]-4,6-diphenoxy-(9CI)
- MF C22 H15 C1 F2 N4 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- MF C29 H23 N9 O15 S4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN Benzoic acid, 2-[[2-(acetylamino)-4-[[7-[[4-[(3-carboxyphenyl)amino]-6-(hexylamino)-1,3,5-triazin-2-yl]amino]-1-hydroxy-3-sulfo-2-naphthalenyl]azo]-5-ethoxyphenyl]azo]-, triammonium salt (9CI)
- MF C43 H43 N11 010 S . 3 H3 N

●3 NH3

- L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN Benzamide, 2-[[4-[(4-bromophenyl)amino]-6-[[[(3-methylphenyl)amino]thioxomethyl]amino]-1,3,5-triazin-2-yl]oxy]- (9CI)
- MF C24 H20 Br N7 O2 S

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IN Benzaldehyde, 3,5-bis[(4,6-dimethoxy-1,3,5-triazin-2-yl)oxy]- (9CI)

MF C17 H16 N6 O7

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzamide, 4-methyl-3-[[4-[methyl(3,3,3-trifluoro-2-methylpropyl)amino]-6-[(3R)-3-pyrrolidinylamino]-1,3,5-triazin-2-yl]amino]- (9CI)

MF C20 H27 F3 N8 O

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN Benzoic acid, 4,4'-[[6-[[4-[[2-[4-(1,1-dimethylethyl)phenoxy]ethoxy]carbon
yl]phenyl]amino]-1,3,5-triazine-2,4-diyl]diimino]bis-, dimethyl ester
(9CI)

MF C38 H38 N6 O7

PAGE 1-B

__Bu−t

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1,3,5-Triazine, 2,4-dimethoxy-6-(3-nitrophenoxy)- (9CI)

09/891,750

MF C11 H10 N4 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN 2-Naphthalenesulfonic acid, 6-amino-5-[[4-[[4-chloro-6-[[3-[[[2-[[2(sulfooxy)ethyl]sulfonyl]ethyl]amino]carbonyl]phenyl]amino]-1,3,5-triazin2-yl]amino]phenyl]azo]-4-hydroxy- (9CI)
- MF C30 H28 C1 N9 O11 S3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN Benzoic acid, 4,4',4''-(1,3,5-triazine-2,4,6-triyltriimino)tris-, tris[3-(pentamethyldisiloxanyl)propyl] ester (9CI)
- MF C48 H78 N6 O9 Si6

PAGE 1-A

PAGE 1-B

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IN 2-Furancarboxaldehyde, 5-(2,4-dichlorophenyl)-, [4-[(3,4-dimethylphenyl)amino]-6-[(4-nitrophenyl)amino]-1,3,5-triazin-2-yl]hydrazone (9CI)

MF C28 H22 C12 N8 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN Benzamide, 3-[(4,6-dichloro-1,3,5-triazin-2-yl)amino]-4-methyl-N-(2-phenylethyl)- (9CI)
- MF C19 H17 C12 N5 O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN Benzoic acid, 4-[[4-[(4-methylphenyl)amino]-6-[[5-(phenylamino)-1,3,4-thiadiazol-2-yl]thio]-1,3,5-triazin-2-yl]amino]- (9CI)
- MF C25 H20 N8 O2 S2

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Benzenesulfonic acid, 4-[[4-[[4-chloro-6-[[4-[[2-ΙN (sulfooxy)ethyl]sulfonyl]phenyl]amino]-1,3,5-triazin-2yl]amino]benzoyl]amino]-, disodium salt (9CI) C24 H21 Cl N6 O10 S3 . 2 Na

MF

●2 Na

PAGE 1-B

__ SO3H

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

Benzamide, 2-[[4-[[(1-naphthalenylamino)thioxomethyl]amino]-6-[(4-phenyl-2-IN thiazolyl)amino]-1,3,5-triazin-2-yl]oxy]- (9CI)

C30 H22 N8 O2 S2 MF

*** FRAGMENT DIAGRAM IS INCOMPLETE ***

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 1,7-Naphthalenedisulfonic acid, 4,4'-[2,4,8,10-tetraoxaspiro[5.5]undecane3,9-diylbis[methyleneimino[6-(4-nitrophenoxy)-1,3,5-triazine-4,2diyl]imino]]bis[5-hydroxy-6-[[3-[(2-hydroxyethyl)sulfonyl]phenyl]azo]-,
tetrasodium salt (9CI)

MF C63 H56 N16 O30 S6 . 4 Na

PAGE 1-B

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzamide, 3-[[4-[(2,2-dimethylpropyl)methylamino]-6-[[(3S)-1-phenyl-3-pyrrolidinyl]amino]-1,3,5-triazin-2-yl]amino]-4-methyl- (9CI)

MF C27 H36 N8 O

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2,7-Naphthalenedisulfonic acid, 5-[[4-[[4-fluoro-6-[[3-sulfo-4-[3-[[2-(sulfooxy)ethyl]sulfonyl]propoxy]phenyl]amino]-1,3,5-triazin-2-yl]amino]benzoyl]amino]-4-hydroxy-3-[(2-sulfophenyl)azo]- (9CI)

MF C37 H33 F N8 O21 S6

PAGE 1-A

HO3SO-CH2-CH2-S-(CH2)3-0

SO3H

NH
OH
HO3S

HO3S

SO3H

PAGE 1-B



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN 2,7-Naphthalenedisulfonic acid, 5-[[4-[[4-[(cyanoamino)carbonyl]-3methylphenyl]amino]-6-fluoro-1,3,5-triazin-2-yl]amino]-4-hydroxy-3-[(1sulfo-2-naphthalenyl)azo]- (9CI)
- MF C32 H22 F N9 O11 S3

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L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C31 H27 C1 N8 O9 S3

PAGE 1-B

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzaldehyde, 4-nitro-, [4-(cyclohexylamino)-6-[(4-nitrophenyl)amino]-1,3,5-triazin-2-yl]hydrazone (9CI)

MF C22 H23 N9 O4

$$O_2N$$
 NH
 NH
 NO_2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN Benzoic acid, 2-[[4-(ethylamino)-6-[(1-methylethyl)amino]-1,3,5-triazin-2-yl]oxy]-, methyl ester (9CI)
- MF C16 H21 N5 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN Benzamide, 3-[[4-amino-6-[(2,2-dimethylpropyl)methylamino]-1,3,5-triazin-2-yl]amino]-N-methoxy-4-methyl- (9CI)
- MF C18 H27 N7 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN 2,7-Naphthalenedisulfonic acid, 3-[[5-[[[4-[(ethenylsulfonyl)methyl]benzoy
1]methylamino]methyl]-2-sulfophenyl]azo]-5-[[4-[[4-fluoro-6(methylphenylamino)-1,3,5-triazin-2-yl]amino]benzoyl]amino]-4-hydroxy(9CI)

MF C45 H38 F N9 O14 S4

PAGE 1-A

PAGE 1-B

-- CH=- CH $_2$

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IN Benzenesulfonic acid, 5-[[4-[(4-acetylphenyl)amino]-6-chloro-1,3,5-triazin-2-yl]amino]-2-[2-(2-sulfophenyl)ethenyl]-, disodium salt (9CI)

MF C25 H20 Cl N5 O7 S2 . 2 Na

2 Na

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzamide, 2-[[4-[[[(2-methylphenyl)amino]thioxomethyl]amino]-6-[(4-phenyl-2-thiazolyl)amino]-1,3,5-triazin-2-yl]oxy]- (9CI)

MF C27 H22 N8 O2 S2

*** FRAGMENT DIAGRAM IS INCOMPLETE ***

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzoic acid, 3,3'-[[6-[[3-(diethylamino)propyl]amino]-1,3,5-triazine-2,4-diyl]bis[imino(6,13-dichloro-4,11-disulfo-10,3-triphenodioxazinediyl)imino[6-[[3-(diethylamino)propyl]amino]-1,3,5-triazine-4,2-diyl]imino]]bis- (9CI)

MF C80 H79 C14 N25 O20 S4

PAGE 1-A

PAGE 1-B

PAGE 1-C

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzamide, 4-methyl-N-(1-methylethyl)-3-[[4-[methyl(2-methylpropyl)amino]-6-[(3R)-3-pyrrolidinylamino]-1,3,5-triazin-2-yl]amino]- (9CI)

MF C23 H36 N8 O

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 1,3,5-Triazine-2,4-diamine, 6-(2-benzothiazolylthio)-N,N'-bis(3nitrophenyl)- (9CI)

MF C22 H14 N8 O4 S2

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IN 1-Naphthalenesulfonic acid, 2-[[6-[[4-chloro-6-[[4-[(cyanoamino)carbonyl]-3-methylphenyl]amino]-1,3,5-triazin-2-yl]amino]-1-hydroxy-3-sulfo-2-naphthalenyl]azo]- (9CI)

MF C32 H22 Cl N9 O8 S2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzoic acid, 3-[[8-[[4-[(3-carboxyphenyl)amino]-6-[(2-hydroxyethyl)amino]-1,3,5-triazin-2-yl]amino]-1-hydroxy-3,6-disulfo-2-naphthalenyl]azo]-, diammonium disodium salt (9CI)

MF C29 H24 N8 O12 S2 . 2 H3 N . 2 Na

●2 NH3

2 Na

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2-Propenal, 2-bromo-3-phenyl-, [4-[(4-nitrophenyl)amino]-6-(phenylamino)1,3,5-triazin-2-yl]hydrazone (9CI)

MF C24 H19 Br N8 O2

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L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2-Propenal, 2-methyl-3-phenyl-, [4-[(2-methylphenyl)amino]-6-[(4-nitrophenyl)amino]-1,3,5-triazin-2-yl]hydrazone (9CI)

MF C26 H24 N8 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN Benzamide, 3-[[4-[(2,2-dimethylpropyl)methylamino]-6-[[(3R)-5-oxo-3-pyrrolidinyl]amino]-1,3,5-triazin-2-yl]amino]-N-methoxy-4-methyl- (9CI) MF C22 H32 N8 O3

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 1-Naphthalenecarboxylic acid, 2-[4-[(4,6-dimethoxy-1,3,5-triazin-2-yl)amino]benzoyl]hydrazide (9CI)

MF C23 H20 N6 O4

PAGE 1-A

PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzoic acid, 4-[[4-chloro-6-[[4-(2-phenylethenyl)-3-sulfophenyl]amino]-1,3,5-triazin-2-yl]amino]-, 1-ethyl ester, monosodium salt (9CI)

MF C26 H22 Cl N5 O5 S . Na

Na

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzoic acid, 2,2'-[1,3-phenylenebis[iminocarbonylimino(6-sulfo-3,1-phenylene)azo(8-sulfo-4,1-naphthalenediyl)imino(6-fluoro-1,3,5-triazine-4,2-diyl)imino]]bis-(9CI)

MF C60 H42 F2 N18 O18 S4

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzoic acid, 3,3'-[[6-[[3-(diethylamino)propyl]amino]-1,3,5-triazine-2,4diyl]bis[imino(6,13-dichloro-4,11-disulfo-10,3triphenodioxazinediyl)imino[6-[methyl(2-sulfoethyl)amino]-1,3,5-triazine4,2-diyl]imino]]bis- (9CI)

MF C72 H61 C14 N23 O26 S6

PAGE 1-B

PAGE 1-C

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzoic acid, 3-[[4-[(4-carboxyphenyl)amino]-6-[(4-chlorophenyl)thio]1,3,5-triazin-2-yl]amino]- (9CI)

MF C23 H16 C1 N5 O4 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN Benzamide, 2-[[4-[(4-bromophenyl)amino]-6-[[[(3-bromophenyl)amino]]]

nitrophenyl)amino]carbonyl]amino]-1,3,5-triazin-2-yl]oxy]- (9CI)

MF C23 H17 Br N8 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

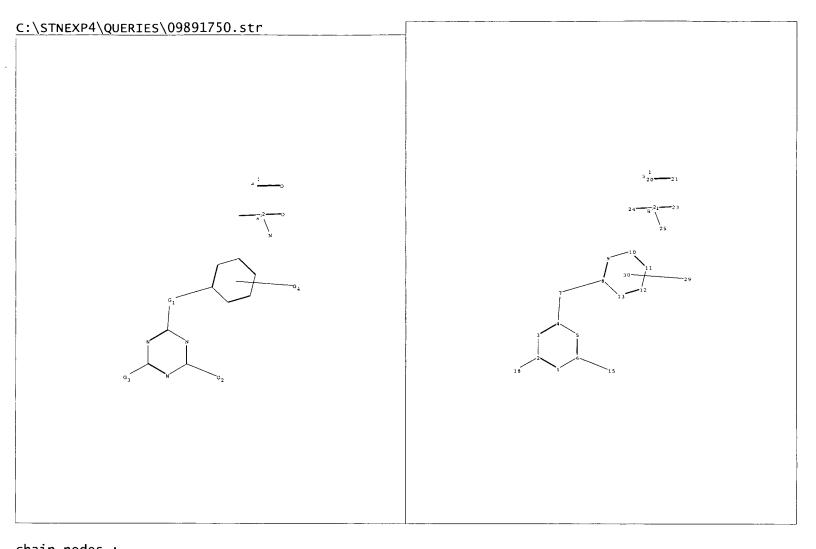
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FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 0.76 0.97

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```
chain nodes :
7 15 18 20 21 22 23 24 25 29 ring nodes :
   1 2 3 4 5 6 8 9 10 11 12
chain bonds :
   2-18 4-7 6-15 7-8 20-21 22-23 22-24 22-25
ring bonds :
   1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-13 9-10 10-11 11-12 12-13
exact/norm bonds :
   2-18 4-7 6-15 7-8 20-21 22-23 22-24 22-25
normalized bonds :
   1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-13 9-10 10-11 11-12 12-13
isolated ring systems :
   containing 8:
G1:0,S,N,CH
G2:X,O,N
G3:0,S,N,X,Cb,Ak
```

G4:NO2,[*1],[*2]

Match level: